

Does SARS-CoV-2 Bind to Human ACE2 Stronger than SARS-CoV?

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Supporting Information for “Does SARS-CoV-2 Bind to Human ACE2 Stronger than SARS-CoV?”

SARS-CoV:	R426 Y436 Y481 Y484 T486 T487 G488 Y491	L472 N473 Y475	Y442 L443 N479
SARS-CoV-2:	R439 Y449 Y496 Q498 T500 N501 G502 Y505	F486 N487 Y489	L455 L456 Q493

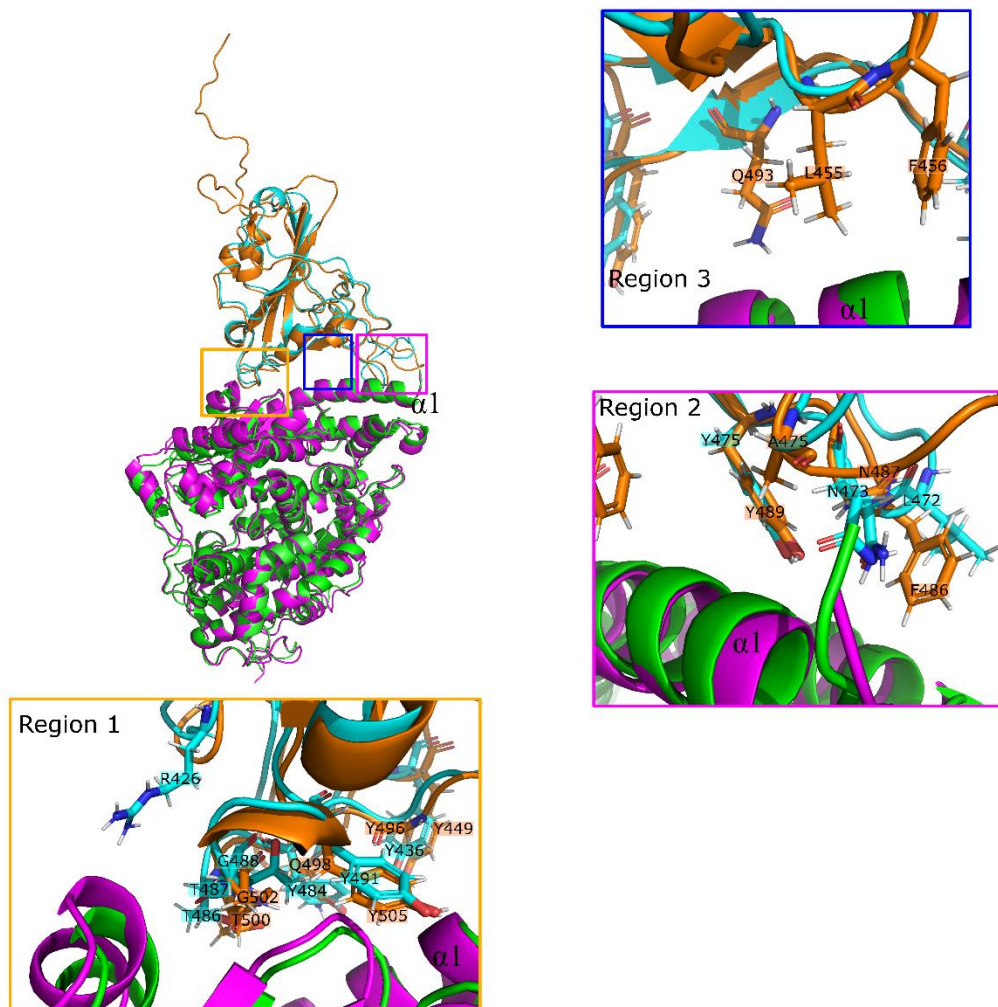


Figure S1: Superimposition of the initial structures of two complexes. The first two lines are a sequence alignment between SARS-CoV and SARS-CoV-2 for the three boxed regions shown below. ACE2-PD in complex with SARS-CoV-RBD and SARS-CoV-2-RBD is highlighted in magenta and green, respectively, and SARS-CoV-RBD and SARS-CoV-2-RBD, cyan and orange, respectively. The residues of the RBD spike proteins that form HB and NBC with ACE2-PD are shown in color boxes.

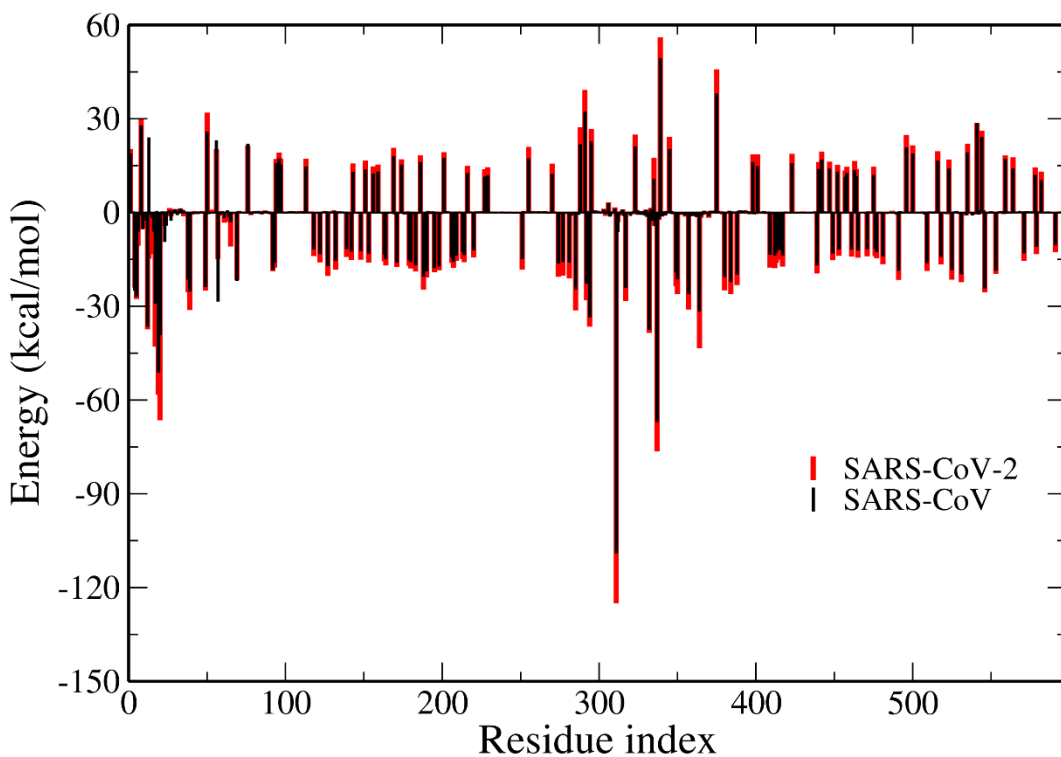


Figure S2: Contributions of the residues of ACE2-PD to the non-bonded interaction energy (kcal/mol). Results were obtained by averaging over 5 trajectories and a window of 0-7000 ns, pulling speed $v=0.5$ nm/s

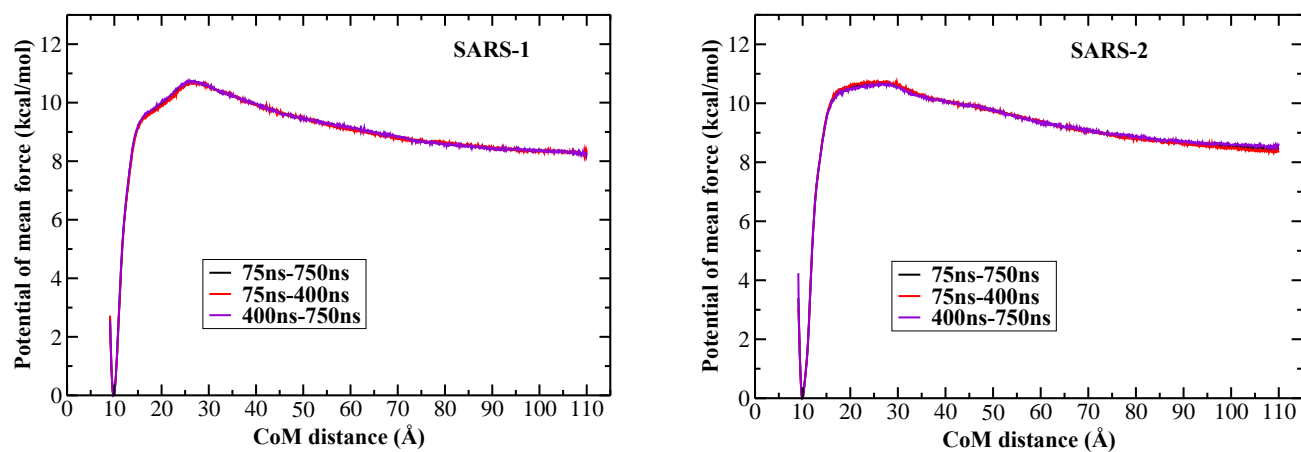


Figure S3: Convergence of REX-US simulations of SARS-Cov (left panel) and SARS-CoV-2 (right panel) through 1D-PMF profiles corresponding to different time windows.